

## CONTENTS

<b>CONTENTS .....</b>	<b>5</b>
List of Figures .....	10
<b>Abstract.....</b>	<b>12</b>
Abstract.....	13
<b>Summary.....</b>	<b>14</b>
<b>CHAPTER 1 .....</b>	<b>17</b>
Chapter 1 Introduction .....	18
1.1 Introduction.....	18
1.2 The Crystal Structure of SmCo <sub>5</sub> .....	19
1.3 Electronic Band Structure Calculation.....	19
1.3.1 The Empirical Pseudo-Potential Method .....	21
1.3.2 The Tight-Binding Method .....	22
1.3.3 The Nearly Free Electron Approximation.....	22
1.4 Electrons in Condensed Matter .....	23
1.5 Ab Initio Calculations Method.....	24
1.6 Application of RE- Permanent Magnets .....	26
<b>References Chapter 1 .....</b>	<b>28</b>
References Chapter 1 .....	29
<b>Chapter 2 .....</b>	<b>33</b>
Chapter 2 Calculation from First Principles.....	34
2- Theory and Computation .....	34
2.1 What is First-Principles Calculation?.....	34
2.2 Density Functional Theory. ....	34
2.2.1 Structure of Matter.....	34
2.2.2 Adiabatic (Born- Oppenheimer) Approximation .....	36
2.2.3 Quantum Many-Body Theory: Hartree-Fock Approximation ...	37
2.2.4 Density Functional Theory .....	39
2.3 Different method of calculating energy bands .....	54
2.3.1 Solving the basis set.....	54
2.3.2 Solving the basis set by (Plane wave) .....	55

2.3.3	The Family of Augmented plane wave method .....	56
2.4	The Eigen Value Problem .....	63
2.6	Self-Consistency .....	66
2.6	The Density of States .....	67
<b>References Chapter 2.....</b>		<b>68</b>
<b>Chapter 3 .....</b>		<b>71</b>
Chapter III Results and Discussion .....		72
3.1	Results and Discussion.....	72
3.1.1	Ferromagnetic BCC Iron.....	72
3.1.2	HCP Neodymium.....	79
3.2	Computation Methods.....	84
3.3	Results and Discussion.....	86
<b>References Chapter 3.....</b>		<b>96</b>
<b>Conclusions.....</b>		<b>100</b>
<b>Arabic Summary .....</b>		<b>103</b>